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14. ABSTRACT While it is common knowledge that ion beams are easily neutralized for both current and charge density using a variety of means, the precise process of neutralization remains unknown. With the increasing importance of electric propulsion, and in particular micropulsion systems, this question is of significant importance. Additionally, it has bearing on thruster design, space instrument calibration, electrodynamic tethers, and ionospheric research. A review of the present state of knowledge on this topic is presented as well as results from ion beam simulations using 2D and 3D Particle-in-Cell (PIC) codes. We investigate both the early "filing" problem of the beam starting to move away from the spacecraft and the steady state problem where the beam encounters a wall at an infinite distance from the spacecraft.					
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INVESTIGATION OF ION BEAM NEUTRALIZATION PROCESSES WITH 2-D AND 3-D PIC SIMULATIONS

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Abstract

While it is common knowledge that ion beams are easily neutralized for both current and charge density using a variety of means, the precise process of neutralization remains unknown. With the increasing importance of electric propulsion, and in particular micropulsion systems, this question is of significant importance. Additionally, it has bearing on thruster design, space instrument calibration, electrodynamic tethers, and ionospheric research. A review of the present state of knowledge on this topic is presented as well as results from ion beam simulations using 2D and 3D Particle-in-Cell (PIC) codes. We investigate both the early “filling” problem of the beam starting to move away from the spacecraft and the steady state problem where the beam encounters a wall at an infinite distance from the spacecraft.

PACS codes:

52.65.Rr Particle-in-Cell Method
 52.75.Di Accelerators and Propulsion
 52.40.-w Plasma interactions
 52.25.-b Plasma Properties

1. Introduction

Ion beam neutralization during operation of electric propulsion devices requires both current and charge density matching with an emitted electron beam. We describe the phenomenon as “current coupling” and note that it is easily accomplished in practice, yet the exact process remains unknown. Currently the neutralization process is described through an “effective collision frequency” that binds electrons to the ion beam. As electric propulsion becomes more prevalent in space missions, this question is of significant importance. Proper modeling of current coupling and neutralization will enable development of low-current neutralizers and optimization of neutralizers for micropulsion devices. Explanation of the effective collision frequency also has bearing on space instrument calibration, electrodynamic tethers, and ionospheric research.

In the early years of electric propulsion research, the ion beam neutralization question was one of the fundamental issues for successful development of this promising technology. A dense ion beam requires space charge neutralization to avoid a potential barrier that can divert or reflect the beam. The vehicle on which the thruster operates needs current-neutrality to avoid excessive charging. In the context of collisionless plasma theory, achieving both current and charge neutrality with the same source of electrons appears to be nearly impossible owing mostly to the large difference in mass between electrons and the ions. For example, define the ion flux, $F_i = N_i v_i$ and the net electron flux, $F_e = \frac{1}{4} N_e v_{et}$ where N is density, v_i is the ion drift velocity, and v_{et} is the electron thermal velocity for a simple effusion model. Achieving both equal density and flux requires $v_{et} = 4v_i$. For example, a 1-keV Xenon beam has $v_i = 38,000$ m/s so a matching electron velocity requires a source temperature of about 0.05 eV; a challenging, but not impossible number. Replacing this simple electron effusion assumption with an injected distribution does not change the misleading picture of a precise balance requirement. A higher temperature, lower density electron source will lead to a positive potential well that does trap electrons, but then the

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theory must explain by what process the trapped electrons shed energy so as to actually fill the well. Another observation is that when ion beams and neutralizers are operated in conducting vacuum tanks, the currents are closely coupled even though the grounding tank eliminates the charge accumulation that could provide feedback for current balance so it appears that one or more plasma mechanisms must be responsible for current coupling.

Possibly first pointed out by L. Spitzer in 1952 [uncited note in Seitz et al. 1961], electric propulsion plumes needed to be properly mixed with electrons or else severe space-charge effects would result. Before the first space tests, there were serious doubts as to the stability of any neutralization approach to the ion beam created by an electrostatic thruster. The general idea was for neutralization to occur shortly after emission to prevent beam return. However, there was lack of understanding as to how the electrons would stay within the beam if they were injected or if the neutralization process was unstable to small perturbations. Failing to properly neutralize the beam would cause a dramatic reduction in thrust, as a significant portion of the beam would return to the spacecraft. This problem was first addressed by the Ramo-Wooldridge staff in their review of electrostatic propulsion in 1960.¹ Their one-dimensional investigation was admittedly unrealistic enough to provide a satisfactory indication as to the stability and practicality of neutralization.

Over the next few years, many theorists who looked at 1- and 2-D models predicted growing instabilities that could turn the beam back to the spacecraft. Some findings pointed towards the possibility of neutralization, such as French's² finding that oscillations in electron current density aided in neutralization or Mirels, (1961)³ who found that emitter location and thermal electrons motion would not significantly impact beam neutralization. Others pointed towards potential problems, such as Seitz et al.⁴ who noted that, if electrons were left to drift into the exhaust beam from a stationary start outside of it, the center of the beam would still develop a virtual cathode and suffer from thrust reduction. Some of the earliest computational studies were brought to bear on the problem, and Buneman and Kooyers⁵, using a one-dimensional PIC code in 1963 were able to provide a neutralized beam when electrons were injected at velocities lower than the directed ion velocity. Fluctuations in the space charge field provided mixing of the beam. Two years later Wadhwa et al.⁶ performed a two-dimensional PIC simulation showing that electrons would oscillate within the beam to allow for neutralization, but theorized that oscillations was not the only mechanism at work. One method suggested was that fluctuations in the space-charge field allowed for entropy increase to mix the electrons, but these fluctuations were not found downstream of the neutralizer.

The 1964 Space Electric Rocket Test I (SERT I) found that it was quite easy to neutralize ion beams in space from a simple neutralizer geometry. In a series of tests it was shown that the ion thruster developed thrust at a level indicating complete beam neutralization. After SERT I, proof of concept was achieved and the theoretical discussion of beam neutralization was dropped in favor of engineering new thrusters. Studies after SERT I include evaluations of neutralizer placement^{7,8}, optimization of the thrusters, and simulations to analyze spacecraft-plume interactions.^{9,10} A few numerical simulations of neutralization have been performed recently, including Othmer et al.^{11,12,13} using a relativistic 3D PIC simulation and Tajmar and Wang investigating FEEP neutralizer placement.¹² Neither proposed a solution to the mechanism of current coupling.

Despite decades of research and the implementation of electric propulsion devices, the detailed process by which an ionized beam is neutralized in space is still unknown. Assorted methods to fit data with theory have been found, but the actual process has yet to be studied in sufficient detail to fully understand the subject. Further, new electric micropulsion devices such as the FEEP or the colloidal thrusters or large arrays of ion and Hall thrusters are still not guaranteed to behave. We might also desire a means to predict and optimize neutralizer operations. Thus, a simulation technique exhibiting beam coupling is needed. Additionally, results from ion beam neutralization modeling will be applicable to ion beams for instrument calibration, electrodynamic tethers, ionospheric research, and fundamental plasma physics.

Our immediate goal is to determine if a standard Particle-In-Cell, PIC, technique is adequate or if additional treatment is needed to understand and capture the current coupling process. We present a series of simulations using a 2-D PIC code^{14,15,16} as well as a 3D PIC/DSMC code.^{17,18} These simulations show the dependence of the beam neutralization on beam energy and neutralization current during the initial "filling" problem and the lack of coupling in the steady-state problem. The simulations presented in this paper serve also as means of validation of the PIC-modules of the 3-D PIC/DSMC code under development.

2. PIC Simulations and Discussion

2-D simulations centered first on examining the dependence of the problem on assorted parameters, such as current density, injection energy, and thermal energy. They also gave a feel for how the system "should" respond in a normal PIC simulation. We examined current-matched and density matched ion and electron beams at different

energies. The domain used for 2-D simulation is shown in Figure 1. In the current-matched cases, the beam stalled while in the density-matched cases the beam propagated without hindrance. Figures 2 and 3 show typical v_x - x phase space plots for these simulations. Parameters for the current-matched and density-matched cases are shown in Table 1. Additional study was performed examining the ion/electron speed ratio. This highlighted that while faster electrons were less likely to neutralize the beam by remaining in the potential well created by the ions, it was not the primary factor. Higher energy beams (1000 eV) neutralized readily even with electrons moving much faster while low energy beams (100 eV) could not be brought to neutralize without an excess of electrons (density matching). Results can be seen in Table 2.

In all cases the majority of electrons were trapped in the potential well created by the ion beam. In current-matched cases, the electrons were unable to fully neutralize the beam and were accelerated to higher energies by the resulting space-charge. The electrons oscillated along the length of the beam, and presumably along other dimensions as well, creating a fairly uniform distribution along the beam. In cases of beam stalling, a distinct “inner core” of electrons can clearly be seen on the phase space plots, as in Figure 2. The front edge was located at the front of the ion beam where the particles were accelerated due to a “surfing” effect from the potential structure. The trailing edge was located along the point of highest potential in the beam, indicating that electrons did not fully return to the injection plane to neutralize the space charge that develops there.

However, one can argue that this filling problem is not what the thruster sees at all, as eventually the end of the beam will fully couple with the background plasma and decouple from the spacecraft. It is certainly not what is seen after more than a few milliseconds in a vacuum chamber as the beam will impinge upon the wall of the chamber or whatever baffling mechanisms are in place. Therefore, the beam would have definite ends on both sides. This makes the bounded problem capable of analyzing which side the electrons exit the problem: we can determine if there is any sort of ion drag that indicates current coupling.

To investigate current coupling six simulations were performed, varying between frozen and unfrozen ions and electron currents at 0.9, 1.0, and 1.1 times the ion current. The base was the unfrozen case at 90% of the ion current. Spreading experienced by the unfrozen ions was the sole observable difference between the simulations. The variation in electron current had no significant impact on the potential of the beam, and all maintained a potential of approximately 3-5% of beam energy.

Using the base case, the total current collected at each end of the simulation was monitored by the code. If the electrons were coupling with the ions, there would be a distinct difference in the current collected at each end as well as a difference between the current collected when the ions were frozen as opposed to unfrozen. Four simulations investigating this scenario were performed, as outlined in Table 4. We initially found that there was a predisposition towards electrons leaving through the right hand side, but this may have been caused by ballistic electrons that begin with enough energy to move across the beam and out the other side without slowing and reflecting. To eliminate this, we began injecting electrons on both sides, each with half the total electron current.

To determine the fraction of electrons leaving the domain on each side, one can develop a simple formula. From current conservation, the current passing through, say, the right electrode is equal to the current from the electron and ion sources as such:

$$I_R = -I_i - I_e^R + f_R^R I_e^R + f_R^L I_e^L, \quad (1)$$

where the subscripts denote the ion or electron current with i and e respectively and the collection side for R . Superscripts denote the injection side. Assuming that the fraction of electrons f leaving each side is equivalent for particles emitted from either side, we can simplify (1) to

$$I_R = -I_i - I_e^R + f_R I_e^T \quad (2)$$

where I_e^T is the total electron current emitted from both sides. Since I_e^R is a component of I_e^T , we can define it as $I_e^R = \beta I_e^T$, so β is the fraction of electrons emitted from the right side. Similarly, the electron current is some fraction α of the ion current, so we can define $I_e^T = \alpha I_i$. This allows us to rewrite (2) as

$$I_R = -I_i - \alpha I_i (\beta - f_r). \quad (3)$$

Solving for f_r , we find

$$f_r = \frac{I_R + I_i}{\alpha I_i} + \beta. \quad (4)$$

Similarly, we find

$$f_L = \frac{I_L - I_i}{\alpha I_i} + \gamma \quad (5)$$

where $f_R + f_L = 1$ and $\beta + \gamma = 1$. A similar solution for f_R and f_L can be found in the case of frozen ions where no ion current is collected. Full current coupling would be indicated by $f_R = 1$ as all the electrons follow the ions out of the problem on the right side. If there is no preference for either side, the ratio f_R/f_L should scale as the ratio of the areas collecting current. The current on the electrode was calculated and recorded over the duration of the simulation and averaged over the entire simulation period, excepting a brief window at the beginning before the electrons had properly mixed.

In XPD2, the current diagnostic is related to the electrode at each end, which also injects particles into the domain. This requirement forced us to perform simulations in both with equal area electrodes at each end and where the right hand side electrode was twice the size of the left hand electrode to accommodate the spreading of the ion beam. This affects the collected currents, as shown above, but does not invalidate the simulations.

As seen in Table 4, we observed no preference for the direction of electrons leaving the simulation when $\beta = 0.5$ in case 4.4, as $f_R \simeq f_L \simeq 0.5$. There seems to be a slight preference for drift out the right in case all cases other than 4.4, but the preference is due to the difference in electrode sizes as it is not affected by freezing or unfreezing the ions. This conclusively demonstrates the lack of current coupling in steady-state PIC simulations.

The role of permeance in beam neutralization remains under investigation. As permeance decreased in the beams, the ability to neutralize the beam dramatically increased. Also looking at the dramatic variance in susceptibility to electron velocity, permeance likely plays a large role in neutralization stability.

The 3-D domain shown in Figure 4 was generated similar to 2-D and the filling problem simulations were performed. Use of a 3-D code to model this essentially 2-D problem was performed as a trial before simulations took on the more physical case with a separate, localized neutralizer. The results obtained match the 2-D simulations closely. A potential well develops as in the 2-D case, as seen in Figure 5. The ion phase space becomes more “rounded” as alternate routes around the potential wells are found as in Figures 6 and 7. Ions accelerated out of the well are also seen in 3-D. A noticeable effect of downstream Neumann (floating) boundary conditions was the escape of newly injected electrons, which could easily reach the downstream boundary and were allowed to escape. Older or original become trapped by the deepening potential well thus creating a very visible “inner core” effect as seen in 2-D. This core could be seen to align its leading edge with the accelerated ion front and the trailing edge with the point of beam reversal, again as seen in 2-D.

3. Conclusions

The inability of the steady state problem to demonstrate current coupling indicates that there are mechanisms happening that are not considered in standard PIC codes. While it can be shown that the currents must match in order to provide a stable start to the ion beam during the initial “filling” problem, by the time the problem reaches steady state there is no mechanism to draw the electrons down the ion beam as simulated in standard PIC. It is clear that the full physics of beam neutralization are not understood at present. Previous work on the subject has been presented without a clear answer. Further development of models and continued study is necessary for a complete understanding of the ion beam neutralization problem.

This series of 2D simulations has demonstrated that what can be called a standard approach to explicit PIC does demonstrate charge neutralization, but not current neutralization. Since the charge neutralization was present in all the runs including those with frozen ions we may conclude that the electrons “fall” into the positive potential well by exchanging energy with other electrons via the action of the electrostatic field. Since the simulations do not exhibit current coupling, we may also conclude that motion of the ions is not inducing any coherent phase velocity into the electrostatic field, i.e. propagating electrostatic waves which would entrain electrons. Since these waves are convecting with the ion beam at a velocity small compared to the electron velocity, the resonant coupling should be weak. Our future work will purposely inject ion density waves to determine what is required for PIC to exhibit this weak coupling, which could be easily suppressed numerically. If, however, we can trust these simulations we can formulate the following hypothesis: either an ion beam couples to its neutralizer electrons due to correlations or structures in the ion population that can induce a down stream phase velocity in the electrostatic field, an effect that can still be modeled with PIC; or the electrons are responding to something like Coulomb collisions on a sub-Debye scale that cannot be captured by PIC.

4. Acknowledgements

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Constant Simulation Parameters					
nc_x	nc_y	L_x	L_y	τ	L_{elec}
128	128	0.05	0.05	1.0E-11	0.025
n_{bg}	W	m_{ion}	E_{xe}	T_i	T_e
1E11	1e4	2.18e-25	0	0.1	0.01
Simulation Variables and Results					
Case	j_i	j_e/j_i	E_{xi}	ϕ_{max}	P
1.1	1.21E+19	1.00	100	111.8380	4.85E-7
1.2	1.21E+19	3.46	100	1.7708	4.85E-7
1.3	3.83E+19	1.00	1000	20.6984	4.85E-8
1.4	3.83E+19	1.09	1000	1.5144	4.85E-8

Table 1: 2-D Simulation parameters and current-density comparison results

Case	Base case	T_e (eV)	V_e (m/s)	V_e/V_i	Virtual Cathode?
2.1	1.5	1.0	419386	10.94	Yes
2.2	1.5	0.1	132621	3.46	No
2.3	1.3	8.36E-4	12123	1.0	Yes
2.4	1.3	2.09E-4	6061.5	0.5	Yes

Table 2: 2-D velocity ratio simulation parameters and results

Case	Ions	β	α	ϕ_{ave} [V]
3.1	Frozen	0	0.9	0.38
3.2	Warm	0	0.9	0.59
3.3	Frozen	0	1.0	0.69
3.4	Warm	0	1.0	1.73
3.5	Frozen	0	1.1	0.50
3.6	Warm	0	1.1	1.53

Table 3: Steady state simulation parameters and results. “Warm” ions indicate the ions were mobile and allowed to develop from a cold beam. “Frozen” ions indicate particles were placed in the problem by the code in a perfectly cold beam.

Simulation #	Ions	β	α	R. Electrode Size	f_L	f_R
4.1	Warm	$\frac{1}{2}$	0.9	2	0.33	0.59
4.2	Cold	$\frac{1}{2}$	0.9	2	0.35	0.61
4.3	Warm	$\frac{1}{2}$	1.0	2	0.32	0.67
4.4	Frozen	$\frac{1}{2}$	1.0	1	0.46	0.49

Table 4: Current coupling simulation parameters and results. “Warm” ions indicate the ions were mobile and started from the developed case 3.2. “Cold” ions indicate the ions were immobile, but started from the developed case 3.2. “Frozen” ions indicates particles were placed in the problem by the code in a cold beam. The right electrode size is in multiples of the left electrode.

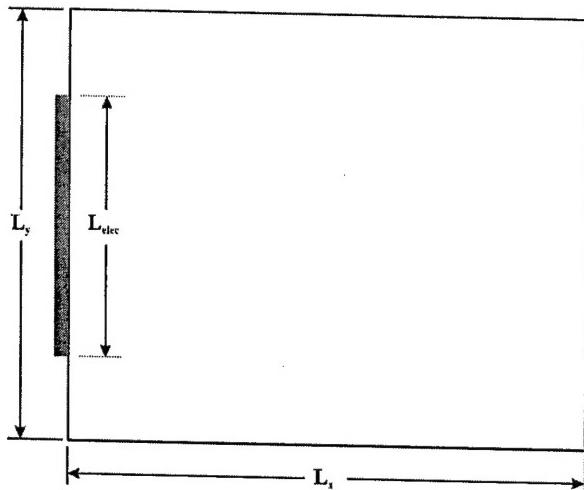


Figure 1: 2-D Simulation Domain

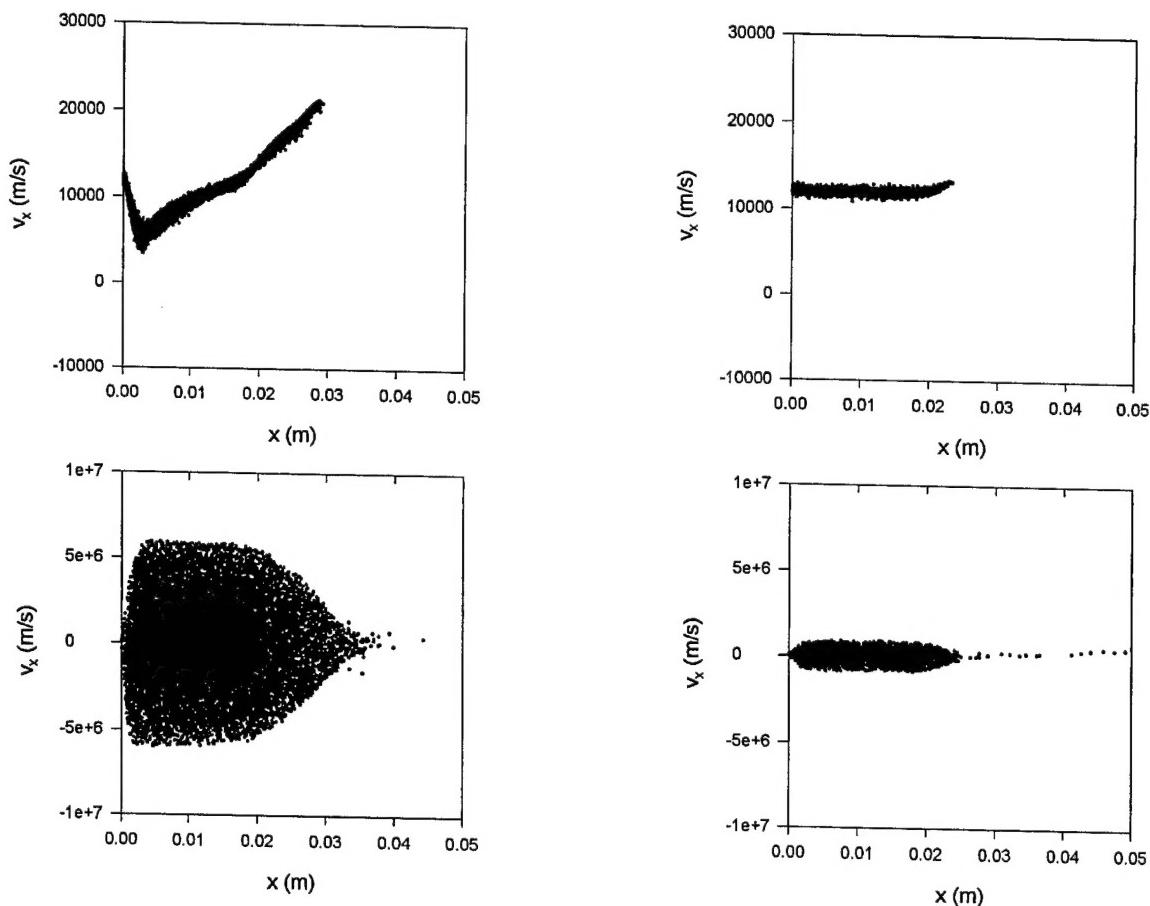


Figure 2: V_x - x phase space plots for 100eV “filling” beam. Left: Current neutralized, case 1.1. Right: Density neutralized, case 1.2. Top: Ion phase space. Bottom: Electron phase space. $t=1.8 \times 10^{-6}$ s

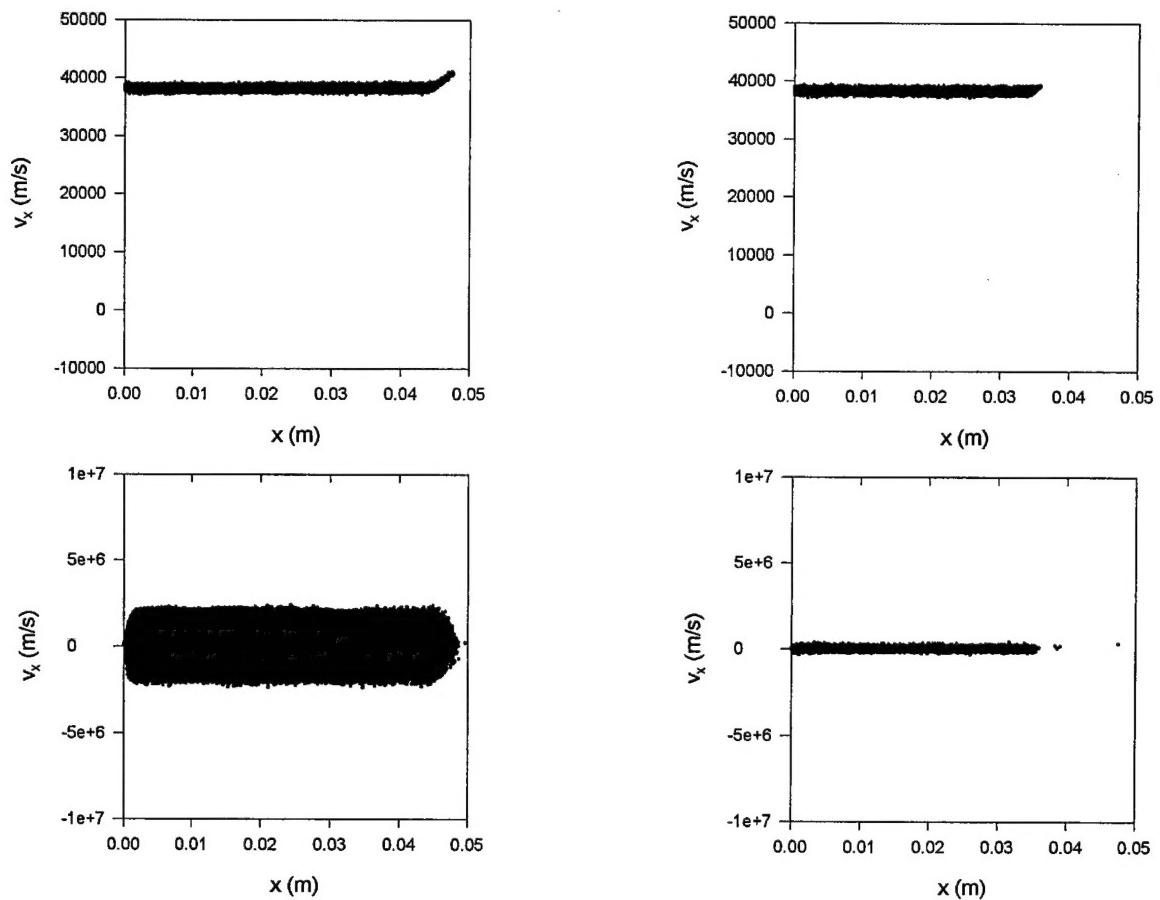


Figure 3: V_x - x phase space plots for 1000eV “filling” beam. Left: Current neutralized, case 1.3. Right: Density neutralized, case 1.4. Top: Ion phase space. Bottom: Electron phase space. $t=1.2\text{e-}6 \text{ s}$

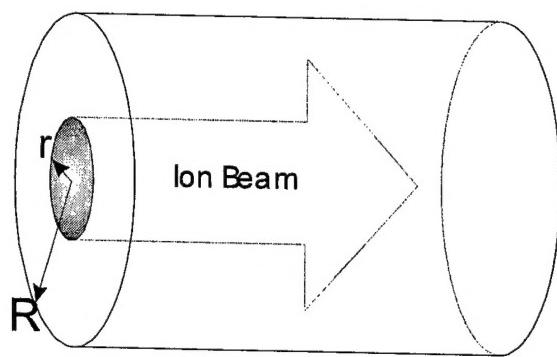


Figure 4: 3-D Simulation Domain

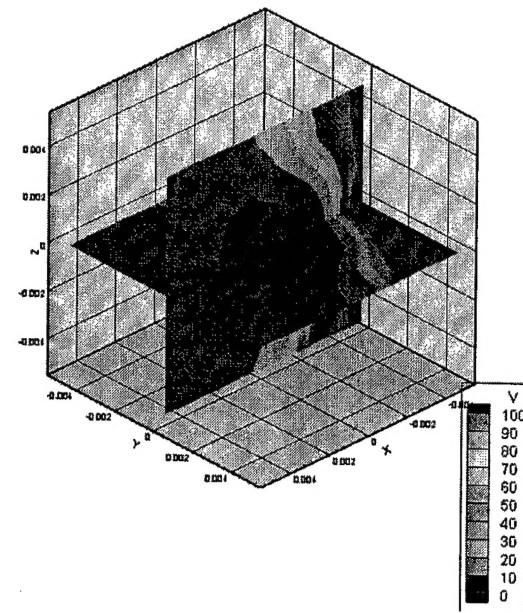


Figure 5: 3-D Potential, $\tau=2.2\text{E-}7$ s

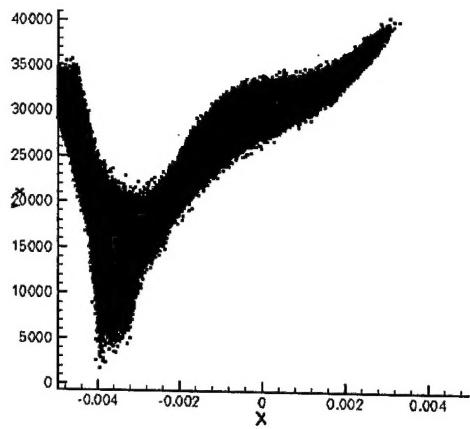


Figure 6: 3-D $V_x - x$ phase space for Ions.
 $\tau=2.2\text{E-}7$ s

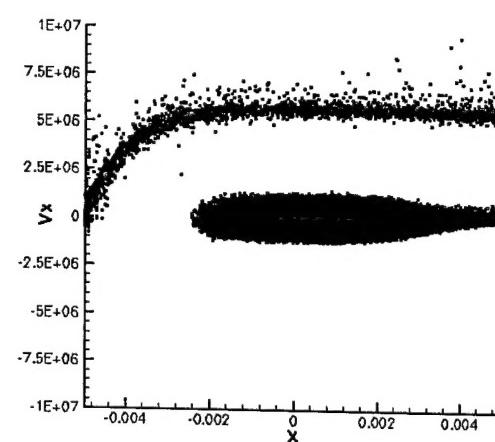


Figure 7: 3-D $V_x - x$ phase space for electrons.
 $\tau=2.2\text{E-}7$ s

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